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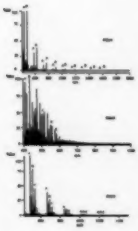
Matrix selection for polymer guanidine analysis by MALDI–TOF MS

Xiaohui Yang, Ting Wu, Bingxiang Liu, Yiping Du, Haiying Li, Shuangliang Zhao, Yunxiang Lu

● Matrix selection for polymer guanidine biocides characterization by MALDI–TOF MS was reported. ● Different matrices were suitable for single polymer guanidines and oxygen-containing polymer guanidines. ● Structural information of three polymer guanidine was analyzed from their best spectra. ● Quantum chemical calculations were carried out to deduce the importance of PA in matrix selection.

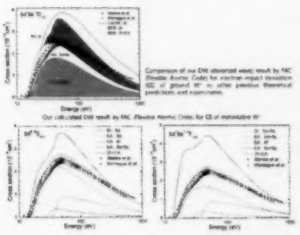


7–13

Electron-impact ionization of W^+ forming W^{2+}

Duck-Hee Kwon, Young-Sik Cho, Young-Ouk Lee

● We have calculated electron-impact ionization cross sections for the ground and metastable levels of W^+ forming W^{2+} using flexible atomic code based on a distorted wave approximation. ● Sensitivity of direct ionization cross section to a single atomic local central potential has been investigated. ● All possible excitation–autoionizations of dipole-allowed $E1$ and non-$E1$, $5d$, $6s \rightarrow nl$ ($5 \le n \le 30$) and $4f$, $5s$, $5p \rightarrow nl$ (n =5,6) are considered with the detailed branching ratios.

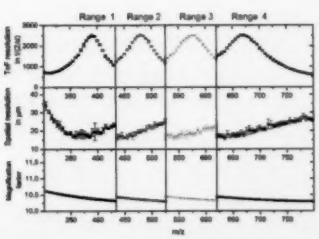


14–23

Velocity corrected ion extraction in microscope mode imaging mass spectrometry

B. Winter, E. Halford, M. Brouard

● Microscope mode imaging mass spectrometry (IMS). ● Application of a velocity corrected ion extraction. ● Tuneable IMS for optimized imaging properties. ● Improved time of flight resolution for linear IMS. ● Imaging samples of up to 5 mm in one experiment.



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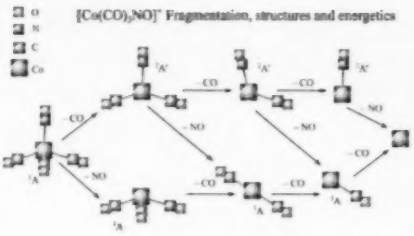
24–32

An experimental and theoretical study on structural parameters and energetics in ionization and dissociation of cobalt tricarbonyl nitrosyl

Peter Papp, Sarah Engmann, Marek Kučera, Michal Stano, Štefan Matejčík, Oddur Ingólfsson

● Experimental and theoretical study on dissociative ionization of cobalt tricarbonyl nitrosyl. ● Structural parameters on the two lowest spin states of $Co(CO)_3NO$, $[Co(CO)_3NO]^+$ and their fragments. ● Appearance energies for sequential ligand loss from $[Co(CO)_3NO]^+$ through dissociative ionization. ● Threshold energies for sequential ligand loss from $[Co(CO)_3NO]^+$ through DFT calculations. ● Theoretical and experimental bond dissociation energies for ligand loss from $[Co(CO)_3NO]^+$.

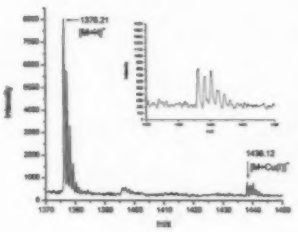


33–36

Preliminary investigation of Cu-containing proteins in seeds of Brazil nuts by ICPMS and MALDI-MS methods

Sarath B. Jayasinghe, Joseph A. Caruso

● Water-soluble protein fraction of Brazil nuts contains Cu-containing proteins. ● A Cu-containing peptide in tryptic digest was identified by MALDI MS using modified isotope pattern. ● A tentative formula, $[M+Cu(I)]^+$, was proposed for the Cu-containing peptide based on MALDI MSd ata.

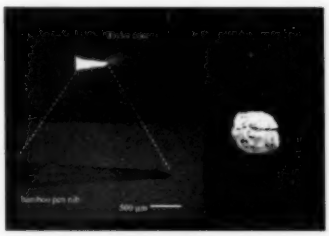


37–40

Electrospray ionization using a bamboo pen nib

Hsin-Kai Chen, Chien-Hung Lin, Ju-Tsung Liu, Cheng-Huang Lin

● This study describes a novel and highly sensitive electrospray ionization method that employs a bamboo pen nib, which is used for the loading and ionization of samples. ● The limit of detection for the analysis of 4-chloroamphetamine can be dramatically improved to 0.01 μg/mL using this technique. ● The results obtained by nib-spray mass spectrometry, wooden-tip mass spectrometry and paper-spray mass spectrometry were compared and findings are discussed.

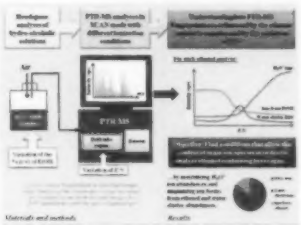


41–45

Modifying PTR-MS operating conditions for quantitative headspace analysis of hydro-alcoholic beverages. 1. Variation of the mean collision energy to control ionization processes occurring during PTR-MS analyses of 10–40% (v/v) ethanol–water solutions

Guillaume Fiches, Isabelle Déléris, Anne Saint-Eve, Brigitte Pollet, Pascal Brunerie, Isabelle Souchon

● Abundances of species from ethanol and of H_3O^+ ions could be controlled. ● *E/N* ratio must be adjusted to the ethanol content to obtain a correct ionization. ● Ethanol fragmentation patterns were reported for *E/N* values from 91 to 512 Td. ● *In vitro* results showed good perspectives for future *in vivo* applications.

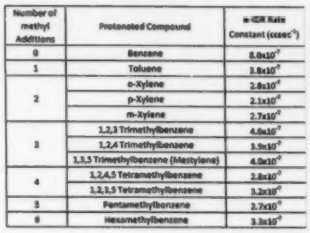


46–48

Electron-ion dissociative recombination rate constants: Effects for benzene analogs with varying degrees of methylation

David Osborne Jr., Nigel G. Adams, Itzhak Dotan

● Addition of a methyl substitution to protonated benzene lowers the rate by ~50%. ● All methyl substitutions greater than one have rate of $\sim 3.2 \times 10^{-7}$cc s^{-1}. ● Number of methyl substitutions has little effect on rate. ● Isomeric form has little effect on the rate.



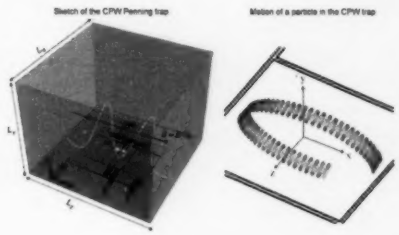
Number of methyl Additions	Protonated Compound	e-IDR Rate Constant (ccsec^{-1})
0	Benzene	8.0×10^{-7}
1	Toluene	3.8×10^{-7}
2	o-Xylene	2.8×10^{-7}
	p-Xylene	2.1×10^{-7}
	m-Xylene	2.7×10^{-7}
3	1,2,3 Trimethylbenzene	4.0×10^{-7}
	1,2,4 Trimethylbenzene	3.9×10^{-7}
	1,3,5 Trimethylbenzene (Mesitylene)	4.0×10^{-7}
4	1,2,4,5 Tetramethylbenzene	2.8×10^{-7}
	1,2,3,5 Tetramethylbenzene	3.2×10^{-7}
5	Pentamethylbenzene	2.7×10^{-7}
6	Hexamethylbenzene	3.3×10^{-7}

49–59

A planar Penning trap with tunable dimensionality of the trapping potential

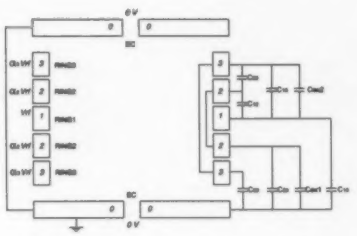
J. Pinder, J. Verdú

● We present a planar Penning trap with tunable dimensionality of the potential. ● The presented planar trap has the magnetic field axis parallel to the surface of the chip. ● We show how to compensate the electrostatic potential. ● We calculate the frequency shifts caused by the magnetic field gradient and curvature in an elliptical Penning trap. ● We discuss one example with a single electron in our planar trap.



60–70

Variable field ion traps

Hrishikesh S. Sonalikar, Atanu K. Mohanty

● We modify a cylindrical ion trap splitting each electrode into several parts. ● The split electrodes are excited by different multiples of a single RF voltage. ● Linear or desired nonlinear field can be obtained by proper choice of amplitudes. ● Increase in field linearity is obtained keeping the simplicity of the CIT. ● Capacitor terminations can generate all required voltages from a single source.